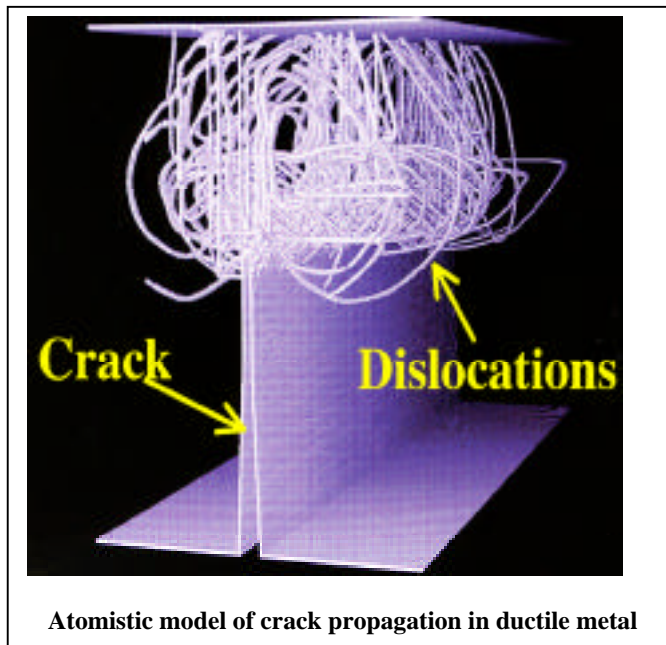


VI.D Computational Simulations of Crack Propagation

Introduction: Cracks happen! Fracture of materials causes structural damage, loss of productivity, and at times, loss of life. However, predicting how and when a material or structure will fail is a difficult task for scientists. Why and how things break involve complex fundamental processes and phenomena occurring on a wide range of length and time scales. Scientists are turning to the largest computers available in order to uncover new clues in solving the mystery of catastrophic materials failure. Laboratory testing of materials can reveal fracture strengths and explore the macroscopic reasons for fracture, but material scientists know that, ultimately, fracture involves breaking bonds between the atoms that make up the solid. Computers are ideal for studying these local, atomistic processes.



Calculational Notes: A simplified model of a metal utilizes Lennard-Jones (LJ) interaction potentials. The figure on the left shows a schematic of a molecular dynamics simulation of an atomistic LJ model with parameters representative of a prototypical ductile fcc structure. The actual calculation contained one billion atoms.

Results: The simulation illustrates some of the complex events that occur as a crack moves in a ductile metal. At first, the crack moves very rapidly and local bonds break in a “brittle” manner, but at some point the crack-tip begins to emit dislocations (the tangles in the picture) and stops propagating. One refers to such a crack as blunted. A blunted crack can cause intense local de-

formation, but it does not cause failure. Cracks that can emit dislocations usually stop before complete structural failure occurs. However, when the material is unable to emit dislocations, crack propagation does not terminate, which eventually leads to failure and irreversible damage of the material. The fundamental phenomena that determine whether a material is able to emit the beneficial dislocations are yet to be elucidated.

Significance: Materials scientists have been studying fracture of metals, alloys, and ceramics for many years. They are still unable to accurately predict when a particular structure may fail. It is possible with large-scale computations, such as the one shown here, to gain new insights into this complex phenomenon. A computer simulation of fracture is able to reveal details at the atomistic scale that cannot directly be observed in experiments. With SSI resources, materials scientists will be able to include needed realism and essential complexity in the fundamental interactions. This will lead to unraveling of the intricate processes that occur as materials catastrophically fail.